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Approximation for Bivariate  
Normal Tolerance Regions**

**Alan H. Feiveson**

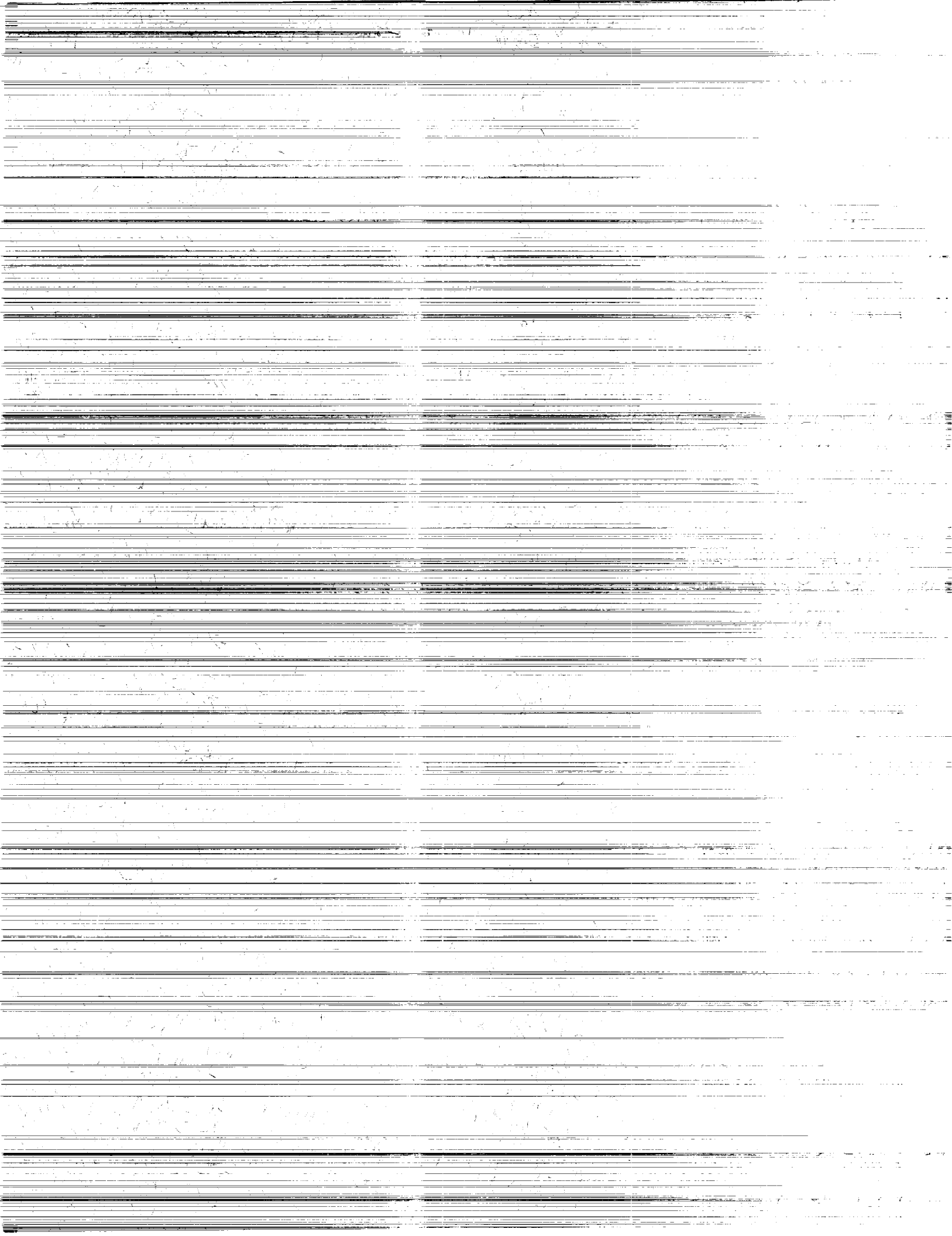
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**Improving the Chi-Squared  
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National Aeronautics and  
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## 1.0 Introduction

Let  $X_1, \dots, X_N$  be a sample of  $N$  observations taken from a bivariate normal distribution with unknown mean vector  $\mu$  and covariance matrix  $\Sigma$ , and let  $\bar{X}$  and  $S$  be the respective  $2 \times 1$  sample mean vector and  $2 \times 2$  sample covariance matrix calculated from the  $X_i$ . Given a desired containment probability  $\beta$  and a level of confidence  $\gamma$ , the problem addressed is to find a region about  $\bar{X}$  that contains at least  $100\beta\%$  of the  $X$ -distribution with probability  $\gamma$ .

When  $S^{-1}$  exists, an ellipse  $R$  about  $\bar{X}$  for any positive number  $c$  may be defined by

$$R = R(\bar{X}, S, c) = \{x: (x - \bar{X})' S^{-1} (x - \bar{X}) \leq c\} \quad (1-1)$$

For a future observation  $X$  distributed according to  $N_2(\mu, \Sigma)$ , the probability that  $X \in R$  is given by

$$I(c) = \frac{1}{2\pi |\Sigma|^{1/2}} \int_R e^{-\frac{1}{2} (x - \bar{X})' \Sigma^{-1} (x - \bar{X})} dx \quad (1-2)$$

For each new sample of  $N$  observations,  $R$ , which depends on  $\bar{X}$  and  $S$ , is a random region in 2-dimensional Euclidean space; thus for a fixed general  $c$ ,  $I(c)$  is a random variable taking values in  $(0, 1)$ . In particular, we seek  $c^*$  (not depending on the unknown  $\mu$  or  $\Sigma$ ), such that

$$P\{I(c^*) \geq \beta\} = \gamma \quad (1-3)$$

The corresponding ellipse  $R(\bar{X}, S, c^*)$ , known as a *tolerance region*, solves the problem.

Based on the work of John (1963) for a general  $p$ -variate normal distribution, the following approximation for  $c^*$  is given by Chew (1966):

$$\tilde{c} = \frac{(N-1) p u'_{\beta}(p, \frac{p}{N})}{\mu_{1-\gamma}((N-1)p)} \quad (1-4)$$

where  $u'_{\beta}(p, \lambda)$  is the  $\beta$ -percentage point of the noncentral chi-squared distribution<sup>1</sup> with  $p$  degrees of freedom and noncentrality parameter  $\lambda$ , and  $u_{1-\gamma}(m)$  is the  $(1-\gamma)$ -percentage point of the central chi-squared distribution with  $m$  degrees of freedom. Equation (1-4) is easier to evaluate than more precise but complicated expressions, such as given by Siotani (1964). Chew states, "the approximation is good if  $1/N^2$  is negligible"; however, it appears (see section 3) that for the bivariate normal case ( $p = 2$ ),  $\tilde{c}$  underestimates  $c^*$  by a factor  $1 - A/N$  where  $A$  depends on  $\beta$  and  $\gamma$ .

For general values of  $p$ , (1-4) has stood the test of time; for example it was cited and used by Rode and Chincilli (1988) in their paper on transforming clinical laboratory measurements. When  $p = 2$ , however, it is feasible to significantly improve the approximation by direct calculation of  $I(c)$  within a Monte-Carlo simulation of values of  $\bar{X}$  and  $S$  (see section 2). Estimation of  $A$  by comparing the resulting more accurate estimates of  $c^*$  with  $\tilde{c}$  makes it feasible to use a corrected form of (1-4) to obtain accurate easily computed tolerance regions.

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<sup>1</sup> Chew defines the noncentrality parameter "in accordance with that in Wilks" (1962); i.e. a noncentral chi-squared random variable with  $m$  degrees of freedom and noncentrality parameter  $\lambda$  is distributed as  $Z^2 + Y$ , where  $Z \sim N(\lambda^{1/2}, 1)$  and  $Y$  has a central chi-squared distribution with  $m-1$  degrees of freedom.

## 2.0 Monte-Carlo Estimation of $c^*$

For  $X \sim N(\mu, \Sigma)$  and any level of confidence, it can be shown that as  $N$  becomes large,  $c^*$  approaches  $c_0 = -2\log(1-\beta)$ . This is because  $c_0$  satisfies

$$P\{(X-\mu)' \Sigma^{-1} (X-\mu) \leq c_0\} = 1 - e^{-\frac{c_0}{2}} = \beta \quad (2-1)$$

(e.g., see Cramér (1963)) and  $\bar{X}$  and  $S$  converge in probability to  $\mu$  and  $\Sigma$  as  $N$  increases. For finite  $N$ , the solution to (1-3) is  $c^* = Kc_0$  for some  $K > 1$ .

Let  $\Sigma^{1/2}$  be a "square-root" of  $\Sigma$  in the sense that  $\Sigma^{1/2}(\Sigma^{1/2})' = \Sigma$ . By making the transformation  $y = \Sigma^{-1/2}(x-\mu)$  in (1-2), it can be shown that the solution to (1-3) is the same as when  $\mu = 0$ ,  $\Sigma = I$  and  $\bar{X}$  and  $S$  are obtained from a sample of  $N$  observations from the  $N(0, I)$ -distribution. As a result, it will be henceforth assumed that  $\mu = 0$  and  $\Sigma = I$ .

For each combination of  $N = 10, 40(5), 50$ ,  $\beta = .90, .95, .99, .999$  and selected values of  $c$  in the range  $c = Kc_0$  ( $1 < K \leq 7.5$ ), 1000 realizations of  $\bar{X}$  and  $S$  were randomly generated taking  $\mu = 0$  and  $\Sigma = I$ . (This can be done without generation of the individual observations; see Odell and Feiveson (1966)). For each  $\bar{X}$  and  $S$ ,  $I(c)$  was then calculated by numerical integration (see appendix).

With  $\beta$  fixed,  $Q(c) = P\{I(c) \geq \beta\}$  is a monotonic increasing function of  $c$ , with  $c^*$  being the root  $Q(c^*) = \gamma$ . From the simulation, for each trial value of  $c$ , say  $c_i$ , the observed proportion of times,  $q_i$ , that  $I(c_i)$  exceeds  $\beta$ , is an estimate of  $Q(c_i)$ . For each  $N$  and  $\beta$ , an interpolating quadratic function was fitted to the points  $(y_i, c_i)$ , where  $y_i = -\log(1-q_i)$ ; ( $.80 \leq q_i \leq .999$ ), then set equal to  $y_\gamma = -\log(1-\gamma)$  to solve for  $\hat{c}_\gamma$ , the estimate of  $c^*$  for  $\gamma = .90, .95$  and  $.99$ . As an example, a plot of  $y_i$  vs  $c_i$  along with the interpolating quadratic function is shown for  $N = 10$  and  $\beta = .99$  in figure 1. The three horizontal lines represent the values of  $y_\gamma$  which define  $\hat{c}_\gamma$ .

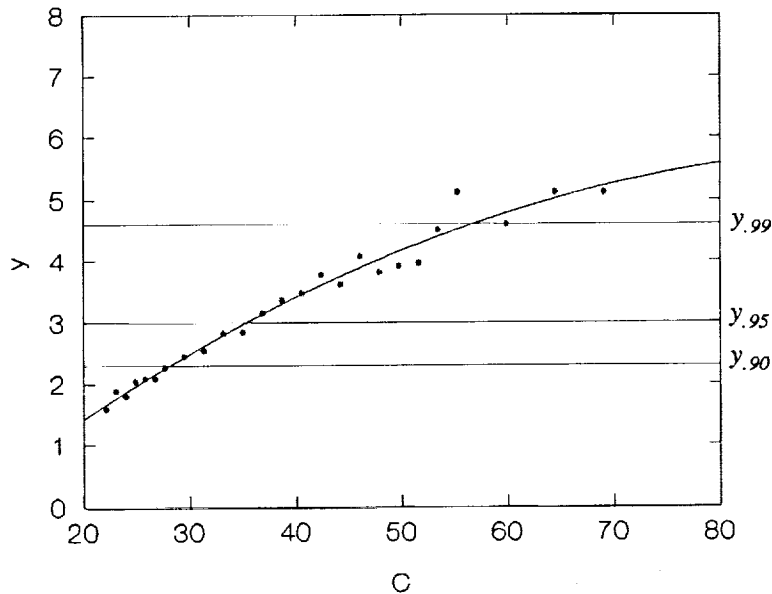


Figure 1.  $y_i = -\log(1-q_i)$  vs  $c_i$  for  $N = 10$ ;  $\beta = .99$

Originally,  $\bar{X}$  and  $S$  were kept fixed as  $c$  was varied for given  $N$  and  $\beta$ ; however, it was noticed that unnatural patterns in plots of  $y$  vs  $c$  would often result. Consequently, it was decided to avoid all dependence between results by regenerating  $\bar{X}$  and  $S$  for each value of  $c$ , despite the extra computational effort.

### 3.0 Accuracy of Point Estimates

The major sources of error in  $\hat{c}_\gamma$  are (1) the numerical integration used to compute  $I(c)$  and (2) the process of fitting an interpolating polynomial to the  $q_i$  and solving for  $\hat{c}$ . A check against the first error was made by using a sufficiently small step size so that values of  $I(c)$  resulted in 1 (to within 5 decimal places) as  $c$  was made arbitrarily large. The second error contains a random component induced by the binomial distribution of the  $q_i$  and some bias due to inverting the estimated  $y$  vs  $c$  relationship as well as possible model error (the true relationship may not be quadratic). Because the obtained fits were so tight (e.g., see fig. 1), the bias in  $\hat{c}_\gamma$  was considered negligible.

To estimate the variance of the random error, a replicate of the entire simulation was made. Under the assumption of constant coefficient of variation, differences between the results were used to estimate a CV of about 1.5% for individual values of  $\hat{c}_\gamma$ . For the final smoothing described below, results of the two runs were averaged, further reducing the error CV by a factor of  $\sqrt{2}$ .

### 4.0 Final Results

Values of  $\hat{c}_{.90}$ ,  $\hat{c}_{.95}$ , and  $\hat{c}_{.99}$  for each  $N$  and  $\beta$  are shown in table 1 along with corresponding values of  $\bar{c}$  obtained from (1-4). A comparison reveals that the latter tend to be smaller by a factor of  $1 - A/N$  where  $A$  depends on  $\beta$  and  $\gamma$ , thus suggesting smoothing the  $\hat{c}_\gamma$  using  $\bar{c}$  as a concomitant variable. Given  $\bar{c}$ , one may then better estimate  $c^*$  by

$$\hat{c}' = \bar{c} [N/(N-A)] \quad (4-1)$$

Using the data in table 1, estimated values of  $A$  for various  $\beta$  and  $\gamma$  were obtained by regression through the origin of  $1 - \bar{c}_\gamma / \hat{c}_\gamma$  against  $1/N$ . These values are shown in table 2. Although there were only eight values of  $N$  for each of the nine regressions, the fits were almost exact. Standard errors of  $A$ -estimates ranged from .04 to .22, corresponding to perturbations in  $\hat{c}'$  between 0.4 and 2.3 percent for  $N = 10$ , and between 0.08 and 0.45 percent for  $N = 50$ . By contrast, errors in uncorrected  $\bar{c}$  are about 50% for  $N = 10$  and 5 - 10% for  $N = 50$ .

**Table 1.** Values of  $\hat{c}_\gamma$  and  $\bar{c}$   
 $\gamma$ -Confidence Tolerance Ellipsoid of Content  $\beta$ ;  
 Bivariate Normal Distribution

$N$	$\beta$	$\gamma = .90$		$\gamma = .95$		$\gamma = .99$	
		$\hat{c}_\gamma$	$\bar{c}_\gamma$	$\hat{c}_\gamma$	$\bar{c}_\gamma$	$\hat{c}_\gamma$	$\bar{c}_\gamma$
10	.900	12.53	8.38	15.45	9.69	24.93	12.97
10	.950	17.07	10.89	21.40	12.60	34.69	16.86
10	.990	28.05	16.72	35.46	19.34	58.85	25.89
10	.999	45.42	25.06	57.25	28.99	91.78	38.81

Table 1 (Cont.), Values of  $\hat{c}_\gamma$  and  $\bar{c}$   
 $\gamma$ -Confidence Tolerance Ellipsoid of Content  $\beta$ ;  
 Bivariate Normal Distribution

$N$	$\beta$	$\gamma = .90$		$\gamma = .95$		$\gamma = .99$	
		$\hat{c}_\gamma$	$\bar{c}_\gamma$	$\hat{c}_\gamma$	$\bar{c}_\gamma$	$\hat{c}_\gamma$	$\bar{c}_\gamma$
15	.900	9.23	7.26	10.68	8.12	14.33	10.13
15	.950	12.47	9.43	14.67	10.56	21.01	13.17
15	.990	20.23	14.50	23.65	16.22	32.80	20.24
15	.999	31.75	21.71	37.90	24.29	52.91	30.31
20	.900	7.91	6.72	8.93	7.38	11.36	8.87
20	.950	10.44	8.74	11.78	9.60	15.09	11.54
20	.990	16.86	13.43	19.20	14.75	25.43	17.74
20	.999	26.57	20.15	30.21	22.14	40.58	26.63
25	.900	7.25	6.39	8.00	6.94	9.95	8.16
25	.950	9.66	8.32	10.68	9.03	13.07	10.61
25	.990	15.31	12.78	17.09	13.88	21.57	16.30
25	.999	24.19	19.19	27.09	20.85	34.43	24.49
30	.900	6.83	6.17	7.45	6.65	8.97	7.68
30	.950	9.04	8.03	9.89	8.65	11.91	9.99
30	.990	14.23	12.34	15.78	13.30	19.65	15.36
30	.999	22.26	18.49	24.58	19.92	30.19	23.01
35	.900	6.53	6.01	7.01	6.44	8.27	7.35
35	.950	8.58	7.82	9.32	8.38	11.11	9.56
35	.990	13.52	12.02	14.65	12.87	17.50	14.69
35	.999	21.33	18.02	23.33	19.29	27.52	22.01
40	.900	6.30	5.89	6.78	6.28	7.91	7.09
40	.950	8.36	7.66	8.98	8.16	10.40	9.23
40	.990	13.14	11.78	14.20	12.55	16.78	14.18
40	.999	20.31	17.67	21.97	18.83	26.04	21.27
50	.900	6.02	5.71	6.42	6.04	7.33	6.73
50	.950	7.90	7.43	8.40	7.86	9.70	8.75
50	.990	12.52	11.43	13.36	12.09	15.40	13.46
50	.999	19.03	17.15	20.41	18.13	23.75	20.19

Table 2. Values of  $A$  for Correcting  
 Non-central Chi-Squared Approximation for  
 Bivariate Normal Tolerance Regions.

$\beta$	$\gamma$		
	0.90	0.95	0.99
0.900	3.153	3.543	4.553
0.950	3.521	3.994	5.103
0.990	4.093	4.606	5.800
0.999	4.725	5.254	6.334

Correction is  $\hat{c}' = \bar{c} [N/(N-A)]$ .

As an example, for  $N = 10$ , a 90%-tolerance region ( $\gamma = .90$ ) that contains at least 99% of the population ( $\beta = .99$ ) is found by first computing the chi-squared approximation (1-4), giving  $\bar{c} = 16.72$ , and then correcting



it with equation (4-1). Table 2 gives  $A = 4.093$ ; hence  $\hat{c}' = 16.72[10/(10 - 4.093)] = 28.31$ . The desired tolerance region is the ellipse  $\{x:(x-\bar{X})'S^{-1}(x-\bar{X}) \leq 28.31\}$ .

## 5.0 Concluding Remarks

This paper has illustrated how Monte-Carlo simulation, along with simple regression modelling, can be used to improve a theoretical approximation for a useful special case. The approximation is easily obtained if one has access (through software or tables) to the percentage points of the central and non-central chi-squared distributions. Correction to more accurate values for bivariate normal tolerance regions is readily accomplished for conventional values of  $\beta$  and  $\gamma$  using the appropriate value of  $A$  in table 2.

If one does not have a ready means of obtaining non-central chi-squared percentage points  $u'_{\beta}(p, \lambda)$ , an approximation given in Abramowitz and Stegun (1966) provides even greater simplification of computation with little loss of accuracy when  $p = 2$ . Abramowitz and Stegun give  $u'_{\beta}(p, \lambda) \approx (1+b)u_{\beta}(p^*)$  where  $p^* = a/(1+b)$ ,  $a = p + \lambda$  and  $b = \lambda/(p + \lambda)$ . Here,  $p = 2$  and  $\lambda = 2/N$ , hence  $1 + b = (N+2)/(N+1)$  and  $p^* = 2(N+1)^2/[N(N+2)] \approx 2$  so that for larger values of  $N$ , one may simply use

$$\begin{aligned} u'_{\beta}(p, \lambda) &\approx \frac{(N+2)}{(N+1)} u_{\beta}(2) \\ &\approx -2 \frac{(N+2)}{(N+1)} \log(1-\beta) \end{aligned} \quad (5-1)$$

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## Appendix

### Obtaining $I(c)$ by Numerical Integration

Equation (1-2) may be rewritten

$$I(c) = \int_{x_{2L}}^{x_{2H}} f(x_2) \int_{g_L(x_2)}^{g_H(x_2)} f(x_1|x_2) dx_1 dx_2 \quad (A-1)$$

where  $f(x_2)$  is the density of  $x_2$ ; i.e.  $N(0,1)$  and  $f(x_1|x_2)$  is the density of the conditional distribution of  $x_1$  given  $x_2$ , which is also standard normal, since  $\Sigma = I$ . The limits  $x_{2H}$  and  $x_{2L}$  are given by  $\bar{X}_2 \pm (cS_{22})^{1/2}$  and for fixed  $x_2$ , the limits of  $x_1$  are given by

$$g_H(x_2), g_L(x_2) = \frac{s_{21}(x_2 - \bar{X}_2) \pm \sqrt{|S| [cS_{22} - (x_2 - \bar{X}_2)^2]}}{S_{22}} \quad (A-2)$$

where  $S = (S_{ij})$ . The inner integral in (A-1) is easily computed as  $\Phi[g_H(x_2)] - \Phi[g_L(x_2)]$  where  $\Phi$  is the standard normal cumulative distribution function for which good approximations are available.







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